4,4'-Diaminostilbene 621-96-5 | DTXSID2022412

٨	/lodel	Per	form	an	Ce
П١	/IUUCI	1 01	IUIII	ıaı	-

Model	Data	

Weighted KNN model

5-fold CV (5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE	
0.81	0.55	0.81	0.54	0.71	0.61	

Model Results

Predicted value: 349 L/kg

Global applicability domain: Inside

Local applicability domain index: 5.75e-01

Confidence level: 7.14e-01

Nearest Neighbors from the Training Set

Image not found
Pentanochlor
Measured: 575
Predicted: 365

Image not found MCPB

Measured: 537 Predicted: 245

Image not found

N-Pentyl N-phenylcarbamate

Measured: 407 Predicted: 375